Tetrachloro($^{13}C_2$)ethene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.33e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.85e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

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Tetrachloroethylene
Measured: 1.21e-03
Predicted: 2.33e-03

Image not found

Trichloroethylene
Measured: 8.37e-03
Predicted: 1.13e-02

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1,1,1,2-Tetrachloroethane
Measured: 6.38e-03
Predicted: 7.46e-03

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Pentachloroethane
Measured: 2.37e-03
Predicted: 2.48e-03